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Droplets of ³He–⁴He mixtures

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Abstract

We study the properties of ³He–⁴He mixture droplets using a phenomenological density functional. The structure of a liquid drop with and without vortices is investigated using Monte Carlo simulations. © 2000 Elsevier Science B.V. All rights reserved.

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Droplets of mixtures provide a unique opportunity to test and enhance our understanding of finite size effects and the effects of boundary on the phase segregation between ³He and ⁴He. The study of liquid-helium mixture droplets has been a subject of great theoretical and experimental interest recently. In this work we present Monte Carlo simulations on the structure of ³He–⁴He mixture droplets with and without vortices.

The total free energy for a liquid-helium mixture of ³He and ⁴He can be expressed as [1] $E = \int (E_3 + E_4 + E_{34}) d\boldsymbol{r}$ with $E_3 = (\hbar^2/2m_{3\mathrm{eff}})\tau_3(\boldsymbol{r}) + d_3|\bar{\nabla}\rho_3(\boldsymbol{r})|^2 + \frac{1}{2}b_3\rho_3(\boldsymbol{r})^2 + \frac{1}{2}c_3'\rho_3(\boldsymbol{r})^2\rho(\boldsymbol{r})^{\gamma_3} + \frac{1}{2}c_3''\rho_3(\boldsymbol{r})^{2+\gamma_3}$, $E_4 = (\hbar^2/2m_4)|\nabla\Psi_4(\boldsymbol{r})|^2 + d_4|\nabla\rho_4(\boldsymbol{r})|^2 + \frac{1}{2}b_3\rho_3(\boldsymbol{r})^2 + \frac{1}{2}c_4\rho_4(\boldsymbol{r})^2\rho(\boldsymbol{r})^{\gamma_4}$, $E_{34} = d_{34}\nabla\rho_3(\boldsymbol{r})\nabla\rho_4(\boldsymbol{r}) + b_{34}\rho_3(\boldsymbol{r})\rho_4(\boldsymbol{r}) + c_{3434}\rho_3(\boldsymbol{r})\rho_4(\boldsymbol{r})\rho(\boldsymbol{r})^{\gamma_{34}}$ where $\rho_i(\boldsymbol{r})$ is the particle density of the ^{i}He, $\rho(\boldsymbol{r})$ is the total density $\rho(\boldsymbol{r}) = \rho_3(\boldsymbol{r}) + \rho_4(\boldsymbol{r})$, and m_i are the atomic masses. The macroscopic wave function of ⁴He is $\Psi_4(\boldsymbol{r}) = \sqrt{\rho_4(\boldsymbol{r})}e^{i\Phi}$. The ³He density-dependent effective mass $\hbar^2/2m_{3\mathrm{eff}} = \hbar^2/2m_3(1 - \rho_3(\boldsymbol{r})/\rho_{3c} - \rho_4(\boldsymbol{r})/\rho_{4c})^2$ is fitted to the experimental pressure dependence in the bulk liquid. In the Thomas–Fermi approximation, the kinetic energy densities of ³He can be expressed as $\tau_3(\boldsymbol{r}) = \frac{3}{5}(3\pi^2)^{2/3}\rho_3(\boldsymbol{r})^{5/3} + \frac{1}{18}(\nabla\rho_3(\boldsymbol{r}))^2/\rho_3(\boldsymbol{r}) + \frac{1}{3}\nabla^2\rho_3(\boldsymbol{r})$.

From this energy functional the structure and energetics of ³He–⁴He mixed drops without vortices have

been studied by means of density functional approach (DFA) [2]. The density distribution of ⁴He and ³He without vortices were obtained by solving a set of coupled self-consistent equations (Euler equations for the energy density). In all these calculations, spherical symmetry is assumed. In the case of dilute Bose gas mixture trapped in a symmetric potential, there exist asymmetric solutions [3]. It is not clear whether these symmetric solutions of ³He–⁴He mixed drops are really ground states of the system. Our calculation also provides the density distribution at finite vorticity for the first time.

Here we directly find out the lowest energy configuration with no symmetry restrictions by means of Monte Carlo techniques through simulated annealing. We approximate the volume integral of the energy functional by a discrete sum. We sample a lattice inside a sphere of radius $2R$ consisting of 40 sites along the diameter, making a total of 33 398 sites. We use the Metropolis algorithm, start our simulation with high temperature, then decrease it to a very low temperature step by step. This is an annealing process and the final configuration should be the lowest energy configuration.

Because of the strong interactions between the helium atoms, the particle number is a very sensitive function of the chemical potential. We thus carry out the simulations with fixed particle numbers.

Fig. 1 shows the density structure of mixed droplets with different particle number. Because the mass of ³He is smaller than ⁴He, its quantum pressure is larger than that of ⁴He. ³He is therefore outside of ⁴He. As can be seen, the structure is symmetric. The average energy

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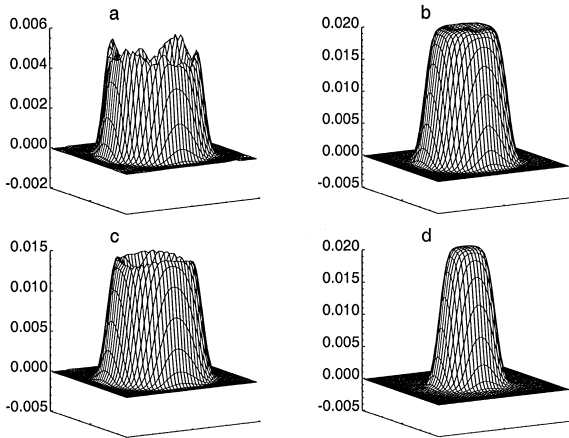
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Fig. 1. Density distributions of ^{3}He (a,c) and ^{4}He (b,d) with particle numbers $N_3 = 1000$ and $N_4 = 3000$ for (a) and (b), $N_3 = 3000$ and $N_4 = 1000$ for (c) and (d).
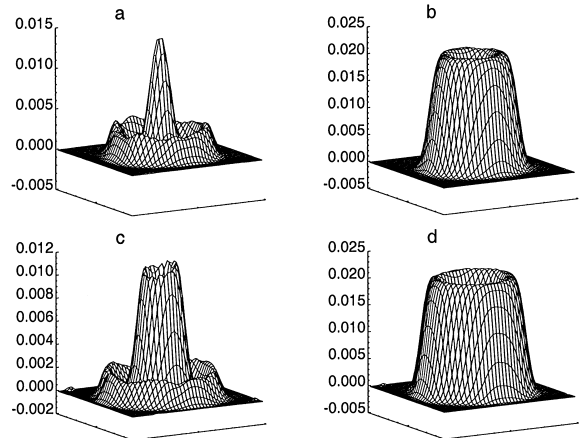

Fig. 2. Density distributions of ^{3}He (a,c) and ^{4}He (b,d) with a vortex in ^{4}He. The vorticity is $m = 1$ for (a) and (b), $m = 7$ for (c) and (d). The particle numbers are: $N_3 = 1000$ and $N_4 = 3000$.

$E/(N_3 + N_4)$ is -5.368 for the case of $N_3 = 1000$, $N_4 = 3000$, and -3.107 for the case of $N_3 = 3000$, $N_4 = 1000$.

The structure is different when there is a vortex in ^{4}He. The density distributions are given by Fig. 2. It shows that ^{3}He will occupy and expand the size of the vortex hole of liquid ^{4}He. At the same time, there are still some ^{3}He atoms on the outside surface of ^{4}He. This comes from an effective attractive potential for ^{3}He on the surface of ^{4}He [4,5]. With high vorticity, the vortex hole of ^{4}He is larger and the surface attraction inside creates a hole in liquid ^{3}He density which is shown in Fig. 2(c).

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